

Theory of the Marginal Fermi Liquid spectrum in the local treatment of the large-U Falicov-Kimball Model.

Mukul S. Laad

*Tata Institute of Fundamental Research,
Homi Bhabha Rd, Colaba, Bombay 400 005, India*

Abstract

The Marginal Fermi Liquid (MFL) hypothesis proposed by Varma *et.al* is derived from a consistent treatment of local spin fluctuations in the Falicov-Kimball (FK) Model. Within an infinite-dimensional mean-field approach, which is exact for this model in $d = \infty$, a marginal Fermi liquid susceptibility and single particle self-energy are obtained near half-filling, and a Fermi liquid phase is recovered sufficiently away from half-filling, in agreement with indications from experiments which probe the normal state of cuprates as a function of doping.

The discovery of high- T_c superconductors in $Cu - O$ based compounds has led to an upsurge of theoretical work concerning the unusual normal state properties of these materials, which appear not to conform to the framework of the Landau Fermi liquid theory [1, 2]. A way of unifying the diverse anomalies observed in experiment was proposed by Varma and coworkers [2], who suggested a phenomenological ansatz for the spectrum of charge and spin fluctuations. For low frequencies $\omega \ll v_F q$ this marginal-Fermi-liquid (MFL) ansatz is

$$Im\chi_{\rho,\sigma}(\omega) \sim \begin{cases} -\rho(0)\frac{\omega}{T}, & \omega \ll T, \\ -\rho(0), & T \ll \omega \ll \omega_c \end{cases} \quad (1)$$

where ω_c is a cut-off energy. The s.p. self-energy $\sigma(\omega) \sim \omega \ln \omega \pm i|\omega|$, as a consequence of (1), and this reconciles the unusual normal state anomalies with the existence of the Luttinger Fermi surface.

As emphasized in [2], the singularities in (1) are in the frequency dependence; the momentum dependence is assumed smooth. In principle, an exact solution of certain strongly correlated models in $d = \infty$, where local fluctuations are treated exactly, should lead to the above spectrum. Furthermore, if these singularities do not depend on any special symmetries which are lost in the lattice problem, they are likely to survive in the lattice problem.

Varma et. al [2, 3] have solved the multiband Hubbard model within the impurity approximation to obtain the MFL form for the local susceptibilities. However, the MFL theory has not been able to account for the T and doping (x) dependence of the Hall constant R_H . Recently, Mahesh et. al [4] have computed the T and x dependence of R_H by numerical diagonalization of the one-band Hubbard model on finite-sized clusters. They were able to account for the anomalous behavior of R_H . However, a proper description of *all* the anomalous features has not been possible, and the extension of the Luttinger liquid [5] concept of Anderson to two dimensions is not clear, unless the small momentum forward scattering couplings become singular [6].

In this letter, we show that a consistent treatment of local fluctuations in the doped, large U Falicov-Kimball model leads to the Eqn. (1). We utilize the exact solution of the infinite dimensional effective Falicov-Kimball (FKM) model [7]. An explicit analytical calculation of the dynamical spin susceptibility $\chi_\sigma(\omega)$ is consistent with the MFL form.

In this paper, the Falicov-Kimball model in 2d in the large U limit,

$$H = -t \sum_{\langle ij \rangle} (c_i^\dagger c_j + h.c) + U \sum_i n_{ic} n_{id} - \mu \sum_i (n_{ic} + n_{id}) \quad (2)$$

is proposed as an effective model capable of describing the anomalous properties of oxide superconductors in their normal state. In this model, t and U should be understood as effective parameters which are determined by comparison of the low-energy spectra of (2) with that of a more realistic three-band model [2,8]. The proposed FKM bears some similarity to the effective model (eqs (12)-(14) of ref. [2]). However, since the authors of ref. [2] solve an impurity model, they require fine-tuning of parameters to reach the critical point. Since we perform a lattice calculation exact in $d = \infty$, the critical behavior survives for a finite range of filling, as the authors of ref. [2] anticipate. In this FKM [7], the d holes are immobile. This means that $[n_{id}, H] = 0 \forall i$; hence, the model has an exact local $U(1)$ symmetry. We notice that the model eqn (2) is different from the usual Hubbard model, which has a global $U(1)$ symmetry associated with *total* fermion number conservation. As we shall see, it is this local symmetry which leads to the breakdown of Fermi liquid theory in our approach.

Since we are interested in the nontrivial local dynamics, we consider an auxiliary impurity model in which the d hole does not hybridize with the “conduction electrons”. This impurity model hamiltonian is the $d = \infty$ counterpart of Eqn. (3), and reads

$$H = \sum_k \varepsilon_k c_k^\dagger c_k + t \sum_k (e^{ik \cdot R_i} c_i^\dagger c_k + h.c) + U n_{ic} n_{id} - \sum_i \mu (n_{ic} + n_{id}) \quad (3)$$

where i represents the impurity site, and k labels the “conduction electrons”. We are interested in the non-trivial local dynamics; hence, we compute the local s.p and two-particle propagators exactly. To compute the s.p Green function, we start with an equation of motion for it.

$$\begin{aligned} (i\omega_\ell + \mu) G_{ii}^c(i\omega_\ell) &= \frac{1}{2\pi} + \sum_k t_k G_{ki}^c(i\omega_\ell) + U \langle \langle n_{id} c_i; c_i^\dagger \rangle \rangle_{i\omega_\ell} \\ (i\omega_\ell + \mu - U) \langle \langle n_{id} c_i; c_i^\dagger \rangle \rangle_{i\omega_\ell} &= \frac{\langle n_{id} \rangle}{2\pi} + \sum_k t_k \langle \langle n_{id} c_k; c_i^\dagger \rangle \rangle_{i\omega_\ell} \end{aligned}$$

$$\begin{aligned}
(i\omega_\ell - \varepsilon_k)G_{ki}^c(i\omega_\ell) &= t_k G_{ii}^c(i\omega_\ell) \\
(i\omega_\ell - \varepsilon_k)\langle\langle n_{id}c_k; c_i^\dagger \rangle\rangle_{i\omega_\ell} &= t_k \langle\langle n_{id}c_i; c_i^\dagger \rangle\rangle_{i\omega_\ell}
\end{aligned} \tag{4}$$

solving for $G_{ii}^c(i\omega_\ell)$ yields (for a Lorentzian unperturbed DOS with a half-width Δ , $\rho_o(z) = (\Delta/\pi)(z^2 + \Delta^2)^{-2}$)

$$G_{ii}^c(i\omega_\ell) = \frac{1}{2\pi} \left[\frac{1 - n_d}{i\omega_\ell + \mu + i\Delta \operatorname{sgn}\omega_\ell} + \frac{n_d}{i\omega_\ell + \mu - U + i\Delta \operatorname{sgn}\omega_\ell} \right] \tag{5a}$$

with the self-energy

$$\Sigma_c(i\omega_\ell) = -\mu + Un_d + \frac{U^2 n_d (1 - n_d)}{i\omega_\ell + \mu - U(1 - n_d) + i\Delta \operatorname{sgn}\omega_\ell} \tag{5b}$$

Also, it is easily seen that

$$\langle\langle n_{id}c_i; c_i^\dagger \rangle\rangle_{i\omega_\ell} = \frac{n_d}{2\pi} \frac{1}{i\omega_\ell + \mu - U + i\Delta \operatorname{sgn}\omega_\ell} \tag{6}$$

The s.p and the two-particle local spectral densities are

$$\rho_c(i\omega_\ell) = \frac{\Delta}{2\pi^2} \left[\frac{1 - n_d}{(i\omega_\ell + \mu)^2 + \Delta^2} + \frac{n_d}{(i\omega_\ell + \mu - U)^2 + \Delta^2} \right] \tag{7}$$

and

$$\rho^{(2)}(i\omega_\ell) = \frac{\Delta}{2\pi^2} \frac{n_d}{(i\omega_\ell + \mu - U)^2 + \Delta^2} \tag{8}$$

From Eqns. (7) and (8), it is clear that the low-energy spectrum is a superposition of s.p and two-particle states. It is precisely the resonant scattering between these states that leads to the breakdown of FLT.

To proceed with the derivation of the MFL spectrum, we compute the NMR relaxation rate, which is related to the low-frequency dynamical local spin susceptibility via

$$\begin{aligned}
\frac{1}{T_1} &= -T \lim_{\omega \rightarrow 0} \sum_{\vec{q}} \frac{\chi''(\vec{q}, \omega)}{\omega}, \quad \text{for } \omega \ll T \\
&= -\sum_{\vec{q}} \chi''(\vec{q}, \omega), \quad \text{for } T \ll \omega.
\end{aligned} \tag{9}$$

where $\chi''(\omega)$ is the imaginary part of the dynamical spin susceptibility. We also have [9]

$$\begin{aligned} \frac{1}{T_1} &= \frac{A^2}{2\hbar N} \sum_i \int_{-\infty}^{+\infty} \langle T_\tau [S_i^+(\tau) S_i^-(0)] \rangle e^{i\omega\tau} d\tau \Big|_{\omega \rightarrow 0} \\ &= \frac{A^2}{2\pi\hbar\Delta N} \sum_i \langle S_i^+ S_i^- \rangle \end{aligned} \quad (10)$$

so that the task reduces to calculating (exactly within $d = \infty$) the local, transverse spin correlation function. This can be computed easily once $\rho^{(2)}(i\omega_\ell)$ is known, by using the identity

$$\langle S_i^+ S_i^- \rangle = \frac{n_d}{2} - \langle n_{ic} n_{id} \rangle \quad (11)$$

But $D = \langle n_{ic} n_{id} \rangle$, the average number of doubly occupied sites is computed directly from the two-particle spectral density via a Matsubara sums

$$\langle n_{ic} n_{id} \rangle = -\frac{1}{\beta} \sum_\ell \rho^{(2)}(i\omega_\ell) e^{-\omega_\ell(-0)} \quad (12)$$

Direct evaluation by use of Eqn. (9) yields

$$\begin{aligned} \langle n_{ic} n_{id} \rangle &= \frac{n_d}{\pi} \left[\frac{\pi}{2} + \tan^{-1} \left(\frac{\mu - U}{\Delta} \right) \right], \quad k_B T \ll \Delta \\ &= \frac{n_d}{\pi} \left[\frac{\pi}{2} + \tanh \left\{ \beta \left(\frac{\mu - U}{2} \right) \right\} \right], \quad k_B T \gg \Delta \end{aligned} \quad (13)$$

Hence from Eqns. (12) and (14), we get

$$\begin{aligned} \langle S_i^+ S_i^- \rangle &= \frac{n_d}{\pi} \tan^{-1} \left(\frac{U n_d}{\Delta} \right), \quad k_B T \ll \Delta \\ &= \frac{n_d}{\pi} \tanh \left(\beta \frac{U n_d}{2} \right), \quad k_B T \gg \Delta \end{aligned} \quad (14)$$

where we used the exact relation $\mu = U(1 - n_d)$. Comparison of Eqn. (10) with Eqn. (11) (after substitution of (15)) leads to

$$\chi''(\omega) = -\frac{A^2}{2\hbar} \rho(0) n_d \tan^{-1} \left(\frac{U n_d}{\Delta} \right) \left(\frac{\omega}{T} \right), \quad \omega \ll T$$

$$= -\frac{A^2}{4\hbar}\rho(0)n_d, \quad \beta U \gg 1, \quad T \ll \omega \quad (15)$$

This is precisely of the MFL form. A second-order perturbative calculation gives $\Sigma(\omega) \sim \omega \ell n \omega - i|\omega|$. Thus, a proper treatment of local spin fluctuations leads to the MFL spectrum for the spin susceptibility as well as the self-energy. It is important to notice that the MFL ansatz is a statement about both the s.p self-energy as well as the susceptibilities, and so approaches which compute only the self-energy of the correct form [10] are inadequate.

Earlier attempts, besides those of [2, 3] have attempted to derive the MFL spectrum by invoking a negative U HM [11], or the Holstein model [12]. The relevance of these models is questionable, since there are no antiferromagnetic insulating or spin fluctuation dominated strange metallic phases in these models. Our approach, which starts from the 2d, Falicov-Kimball model with large U , explicitly takes AFM local spin fluctuations into account. In fact, noticing that the FKM in $d = \infty$ is the recoilless x-ray edge problem [13], the local “excitonic”, or the transverse spin-spin correlation function is divergent at low energy near $n = 1$,

$$\begin{aligned} \chi^{\pm''}(\omega) &= \int_0^\infty d\tau e^{i\omega\tau} \langle T_\tau [S^+(\tau) S^-(0)] \rangle \\ &\sim |\omega|^{-\beta} \end{aligned} \quad (16)$$

with $\beta = \frac{2\delta}{\pi} - \left(\frac{\delta}{\pi}\right)^2$ and $\delta = \tan^{-1}\left(\frac{U}{\Delta}\right)$, the s-wave phase shift at μ . This leads to a soft, local spin fluctuation mode at low energy, and it is precisely the coupling of the s.p part of the spectrum to these soft modes which leads to the MFL ansatz.

The MFL ansatz reconciles the normal state anomalies observed in cuprates with the existence of the Luttinger Fermi surface. We have shown that the MFL ansatz can be derived from a Falicov-Kimball model. Large U is crucial to the derivation, as is the filling factor. The MFL state is unstable to a Fermi liquid (FL) phase for $n < n_c = 1 - \frac{1}{\pi} \cot^{-1}\left(\frac{U}{2\Delta}\right)$ [13]. With $U = 2\Delta$, for e.g., $n_c = 0.75$, i.e. the doping concentration of holes $x = 0.25$, close to the experimental x_c value beyond which the anomalous behavior is suppressed [14]. At lower densities, effects of disorder will introduce qualitatively new

features. A non-perturbative treatment including effects of disorder will be reported elsewhere.

We have not dealt with the superconducting phase in this paper; however, a few remarks can be made. Due to large U , the on site pairing amplitude is severely suppressed, $\langle c_i^\dagger d_i^\dagger \rangle \equiv 0$ (actually, because the Hamiltonian has an exact local U(1) symmetry, this is rigorously true, by Elitzur's theorem). This implies, upon Fourier transforming, that

$$\sum_{\vec{k}} \langle c^\dagger(\vec{k}) d^\dagger(-\vec{k}) \rangle = 0 \quad (17)$$

As pointed out by various authors [15, 16], the pair wave-function should have lines or points on the FS at which it is zero, and hence the pairing is *not* of the BCS variety. The gap function has nodes at the same points where the pair wave function does. It is not possible, from the above, to specify whether the symmetry of the SC state is of the extended s-wave or the d-wave type. This is beyond the scope of the present work.

In conclusion, we have shown that an exact treatment of the dynamical spin fluctuations in the large U , one band Falicov-Kimball model leads to the MFL phase near half-fillings and a FL phase sufficiently away from $n = 1$.

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